Computationally Engineered Microstructural Complexity in Ferroelectric Systems MURI

ARO Materials Sciences Division

California Institute of Technology

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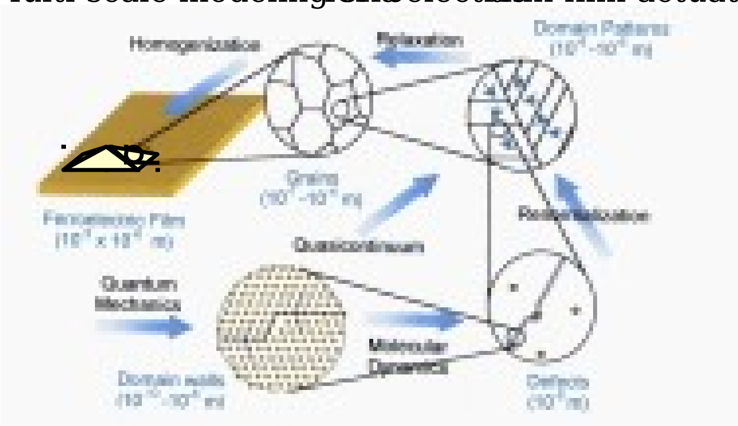
Major Participants

California Institute of Technology

- Mechanical Engineering
- Applied Mechanics
- Chemistry & Applied Physics
- Applied Physics & Materials Science
- Mechanical Engineering
- Mechanical Engineering .& Applied Physics
- Aeronautics
- Materials Science

www.me.caltech.edu/ferromuri

Multi-scale modeling for a ferroelectric thin-film actuator



Objective:

The objective of this research is to extend our ability to computationally treat the complexities found in real materials systems. Specifically, it addresses very fundamental issues related to multi-scale modeling of the microstructure and actuation properties of thin-film ferroelectrics, notably the solid solution system of lead barium titanate (PBT).

Army Relevance:

- Develop the capability to theoretically predict the behavior of ferroelectric materials which are being broadly applied as dielectrics, electronic memories, optical nonlinear elements and actuator applications
- Establish a materials-by-design methodology that will shorten procurement cycles for future Army systems by incorporating multi-scale, multi-phenomenon modeling of materials during their early stages of development

Approach:

% Investigate multiscale modeling of microstructural evolution and its affect on mechanical behavior

% Develop an approach for the deposition of highly tex thin films on silicon substrates

% Characterize domain wall structure and mobility und electromechanical fields

% Optimize the design and performance of a PBT thin-fi microelectromechanical (MEMS) actuator to obtain 5% str

% Design a micropump and an array of microactuators using thin-film ferroelectrics